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ABSTRACT

The first part of this paper addresses the following topics: (1) the usefulness of microcomputers; (2) applications for microcomputers in analytical chemistry; (3) costs; (4) major microcomputer systems and subsystems; and (5) which microcomputer to buy. Following these brief comments, the major focus of the paper is devoted to a discussion of three applications for microcomputers developed at a specific community college: (1) an automatic titrator; (2) a gamma scintillation spectrometer; and (3) a chromatographic data analyzer. (JN)

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# MICROCOMPUTER APPLICATIONS IN ANALYTICAL CHEMISTRY

by Joseph W. Long

In the first half of this paper, I would like to deal with microcomputers in a general way by making comments on the following questions.

1. Why bother with microcomputers at all?
2. What applications are there for microcomputers in analytical chemistry?
3. How much does a usable microcomputer system cost?
4. What are the major systems and subsystems in a microcomputer?
5. Which microcomputer to buy?
6. Where can one get further information on microcomputers?

In the second half of the paper, I would like to briefly describe a microcomputer-controlled automatic titrator which I have assembled, and which is currently being used by students at Broome Community College.

## PART I

### WHY BOTHER WITH MICROCOMPUTERS?

Microcomputers are not toys. Many of today's microcomputers are more powerful and usable than large-system computers from twenty years ago. Over the past few years, the cost of small-system computers has fallen to the point where it is below the cost of much of the instrumentation within even a very modestly equipped analytical laboratory. Computers are finally affordable within many community college chemistry departments. Further, industrial laboratories are making heavy use of microcomputers and our students need some familiarity with this sort of equipment if their education is to remain current. Finally, many of the applications which can be made within an analytical lab can not be done on a large-system computer because of problems related to time-sharing on large systems.

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## WHAT APPLICATIONS ARE THERE FOR MICROCOMPUTERS IN ANALYTICAL CHEMISTRY?

1. They can be used for "off line" data processing. A large-system computer would often (but not always) be a better choice for this application.
2. They can be used for "on line" data processing. Here, data are transferred directly from an instrument to a computer and the data can be processed as the experiment is under way.
3. They can be used for process control. In this case, the computer functions as an executive which, on the basis of a program and perhaps real time data, controls an experiment. The automatic titrator constructed at Broome Community College is an example of this application.
4. They can be used to substitute software (i.e., computer programs) for hardware---electronic components, gears, etc. Examples of this are use of a computer program to generate voltage ramps for use in polarography or to generate pulses to drive a strip chart recorder at different speeds.
5. They can be used for storage of data. The scintillation spectrometer system described later can put 65 spectra on a single minifloppy disk.

## HOW MUCH DOES A USABLE MICROCOMPUTER SYSTEM COST?

Complete microcomputers may be purchased for as little as two hundred dollars or for as much money as one might care to spend. Investing around four thousand dollars is required for a truly high quality, usable system. This investment would include about two thousand dollars for a video terminal, and a good printing terminal. Careful shopping, and deletion of some desirable but not mandatory features, would permit a system to be implemented for about two thousand dollars.

## WHAT ARE THE MAJOR SYSTEMS AND SUBSYSTEMS IN A MICROCOMPUTER?

A microcomputer, like any computer, must have the following systems: a control processor (CPU), memory, some sort of input/output (I/O) and mass storage. In order to be usable for real time processing and control, two additional systems are required. These are a "Controller" and an Analog-to-Digital——Digital-to-Analog converter (AD/DA). The Controller allows relays to be opened or closed in the external world under computer control, and the AD/DA provides a path for analog voltages into and out of the computer.

## WHICH MICROCOMPUTER TO BUY?

An important decision which must be made very early is on which of two approaches to take in setting up a microcomputer. This decision is on whether to buy a complete "one-box" computer or to buy a more modular system. This is analogous to the decision facing the purchaser of high fidelity equipment who must decide on whether to opt for a "components" system, or for a console system. Each has its advantages; but, because of the versatility and expandability it allows, a modular approach seems to be the best approach where process control and real time computing are involved. We have used this approach at Broome Community College with great success. Our microcomputers are all based on the so-called S-100 Bus. S-100 based computers are available from numerous manufacturers, and dozens of other manufacturers produce scores of different boards which will plug right in. The resulting versatility is almost limitless.

## PART II

In this section, I will briefly describe three applications for microcomputers I have developed at Broome Community College. They are:

A. an automatic titrator
B. a gamma scintillation spectrometer
C. a chromatographic data analyser.

A. Microcomputer Controlled Automatic Titrator

The automatic titrator I will describe here illustrates most of the ways in which microcomputers can be applied within the field of analytical chemistry. For that reason, it is a good, concrete example of many of the principles expressed in Part I of this paper. I will discuss the automatic titrator from the following viewpoints:

1. operation of the titrator
2. it's capabilities and applications
3. special (non-computer) hardware required
4. titrator software

## OPERATION OF THE TITRATOR

The titrator consists of a titrant pump and motor (digital burette), a pH meter and a strip chart recorder interconnected through the microcomputer. It functions, briefly, in the following way: the computer monitors the pH of the solution being titrated. When the pH reaches a constant value, it is output to the teletype and to the chart recorder. Under computer control, the chart recorder paper is advanced, a titrant increment is added and the cycle begins again as the computer monitors the pH of the solution once more.

## TITRATOR CAPABILITIES AND APPLICATIONS

(a) It can perform any potentiometric titration which could be done manually using a standard pH/millivolt meter, including acid-base, redox precipitation titrations, etc.

(b) As each increment of titrant is added by the computer-controlled pump, the pH (or voltage) can be printed on a teletype. At the same time, the data can be plotted under computer control on a strip chart recorder.

(c) Titrating variables, such as the amount of titrant to be delivered, chart recorder format, criteria for stopping the titration, etc. are set by the operator in response to prompts from the titrator program.

(d) Changes in the software allow limitless modification and adaptation of the titrator's capabilities. For example, first or second derivative plots can be done, or routines to perform stoichiometric calculations based on the endpoint of the titration could be added. This can be done by changing the titrator programs. The hardware need not be touched. Here is an excellent example of replacement of hardware. Operational amplifiers would be required for derivative plots if the programming power of the computer were not available. This makes the titrator very versatile and in many ways, "intelligent."

## TITRATOR SOFTWARE

The titrator program is written in a special form of BASIC called "CONTROL BASIC" which is especially designed for process control. Figures B and C give a flow diagram and titration curve generated by the titrator. Once the system is started, the sample is titrated and the curve plotted completely automatically.

# AUTOMATIC TITRATOR

Red arrows indicate direction of data flow

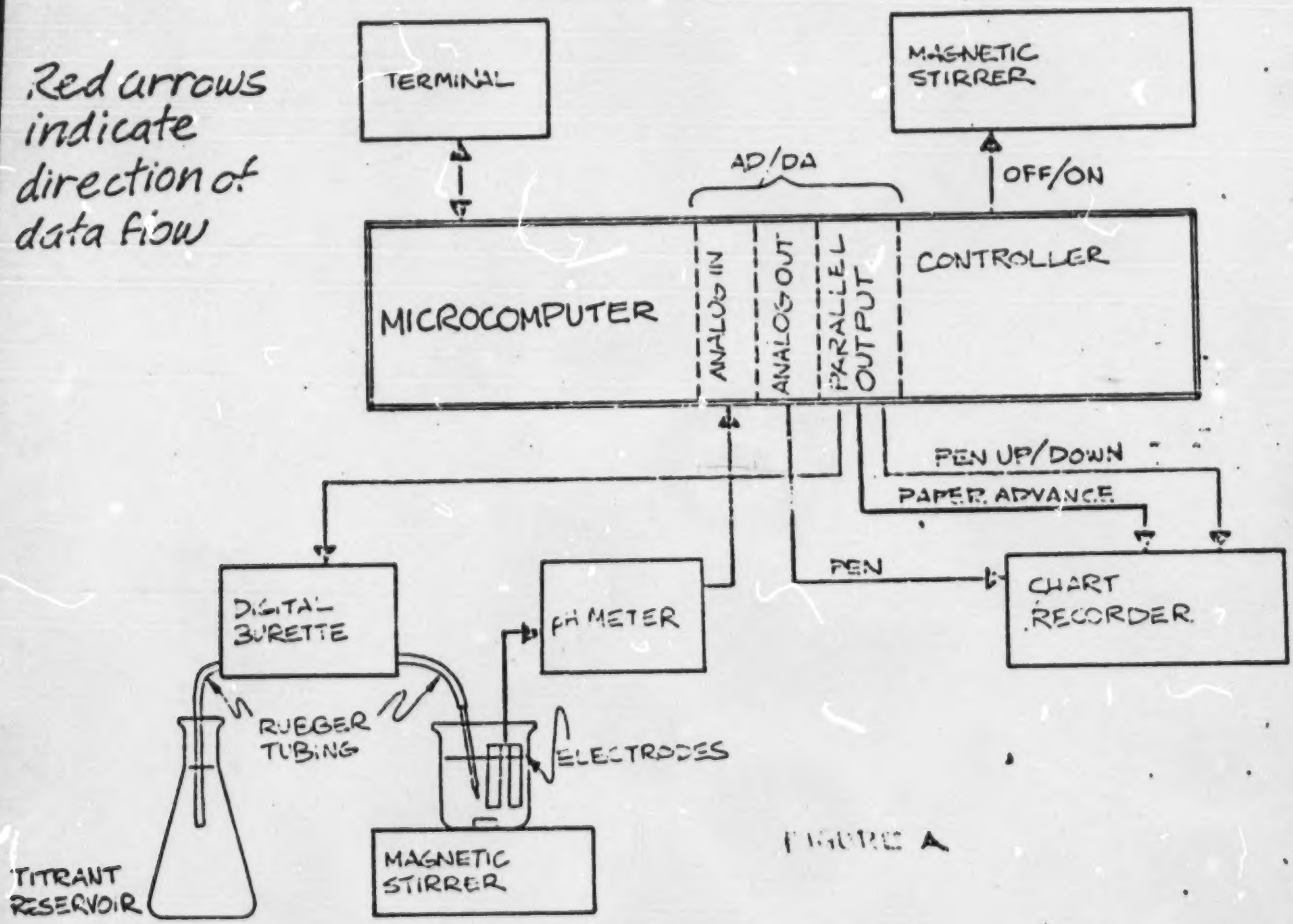



FIGURE A

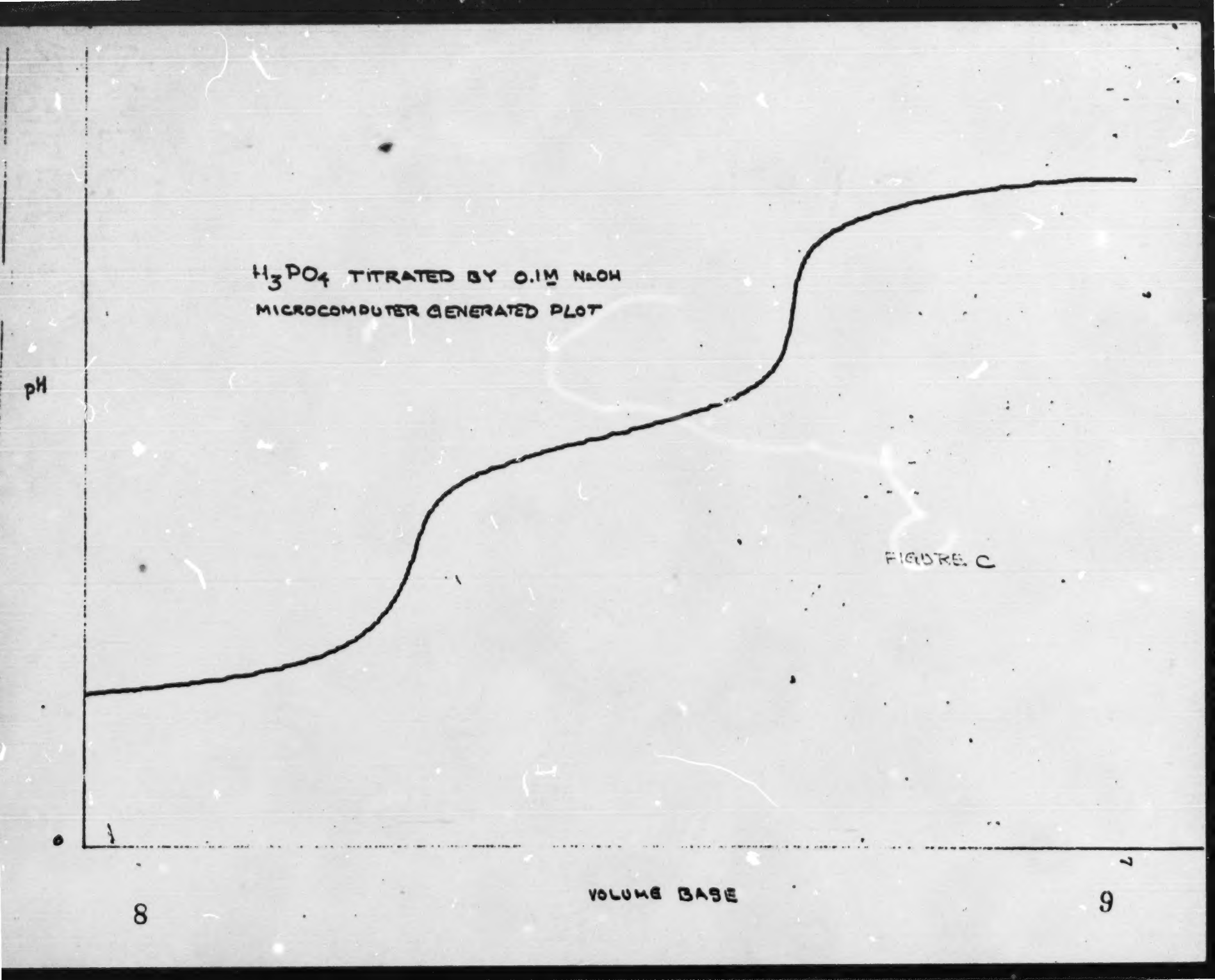

$H_3PO_4$ TITRATED BY 0.1M NaOH
MICROCOMPUTER GENERATED PLOT
pH
VOLUME BASE

FIGURE C

# INSTRUCTIONS FOR OPERATION OF THE PROCESSOR TECHNOLOGY GAS CHROMATOGRAPHY DATA ANALYSER

## I. INTRODUCTION

### A. Capabilities

This equipment will analyse the results of gas chromatographic runs and produce the following information:

1. relative area of each peak
2. retention time of each peak.

The information is automatically output to a printer if hard copy of the data is desired.

### B. Limitations

The analyser makes the following assumptions about the chromatographic data:

1. The baseline is constant and close to zero.
2. The data are fairly noise-free.
3. The peaks are completely resolved.
4. The peaks are symmetrical. (Affects accuracy of retention time only.)
5. The peaks are of reasonable height on a 10 mV scale recorder.

Assumptions 1—4 are based on the analyser software, which could be modified to eliminate any or all of them.

Assumption 5 is based on the analyser hardware and would require modification of the "analog and digital interface" described below.

### C. Hardware Description

The equipment consists of a processor technology microcomputer system, including a dual floppy disk, AD/DA converter, video display and printer.

The interface between the computer and chromatograph is another piece of hardware called an "analog and digital interface". This box connects the chromatograph to the computer. Its purpose is to convert the output voltage level of the GC into a level and range usable by the computer.

Figure 1 is a diagram of the hardware.

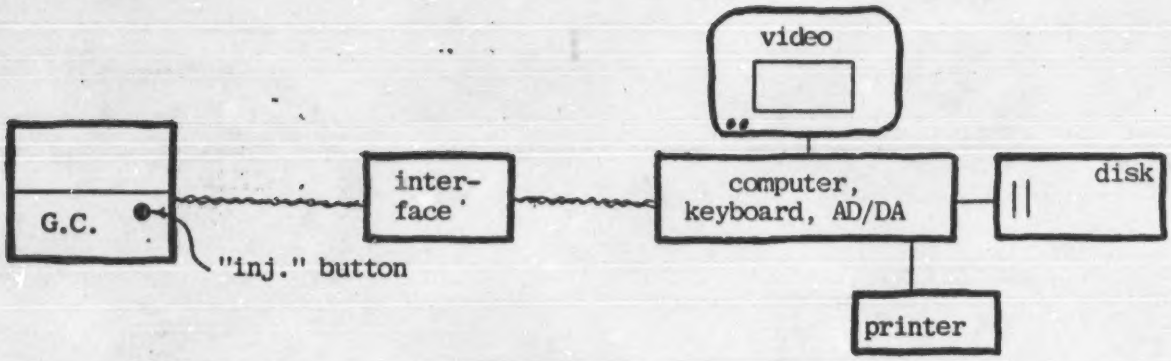



FIGURE 1

## II. START-UP AND OPERATION

### A. GC Start-Up

1. Start up GC in normal manner.
2. Adjust sample size to give good peaks when recorder is set to 10 mV scale.
3. Carefully zero recorder, using recorder zero adjust and zero button.
4. Adjust GC filament current to exactly zero on recorder.
5. Turn on "analog and digital computer interface."

### B. Computer (cold) Start-Up

1. Turn on computer (key on disk). You should see a > prompt on video display.
2. Carefully insert disk into L.H. drive. Be sure disk is oriented correctly.
3. Type: boot <ret> . You should get a "PTDOS" message, followed by a star (*) prompt.
4. In response to *, type: DO INTEG <ret> .
5. The analyser software will load and automatically execute.
6. You should see the following prompt: "Number of peaks expected?"
7. If you got this far, all is well. If not, remove disk, turn off computer and go to B-1.

### C. Operation of Analyser Program

1. Touching the "mode select" key will stop the program. Type: RUN to start it again.
2. Advice on response to various prompts in program.
   a. "Number of peaks expected?" Enter the number if you know; otherwise enter a large number (say, 1ØØ).

b. "Do you want hard copy?" Enter yes or no, as it pleases you.
c. "Turn on TTY." Be sure local light (on keyboard) is off.
   (1) Turn TTY to line, not local.
   (2) Local light is on lower left of keyboard. Try pushing the key a few times.

D. "Type 'GO' as you inject sample."

At this point, your sample should be in syringe, ready to inject. As you inject, push inject button (on lower GC box).

E. "Touch escape key to interrupt and print results early."

1. Escape key is in upper L.H. corner of keyboard.
2. Use escape key if you see all the peaks you want analyzed. Useful when you don't know in advance how many peaks to expect.

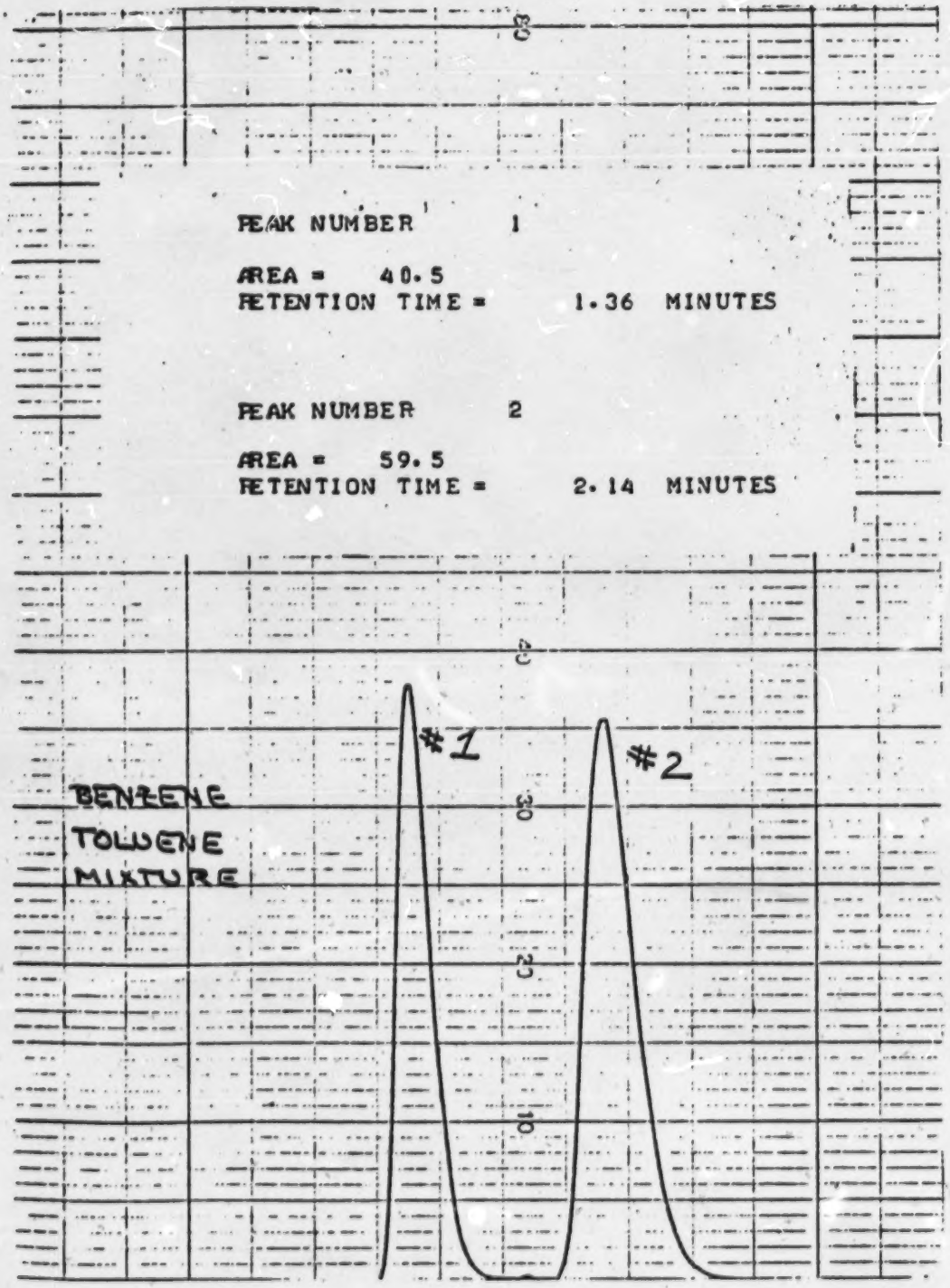
F. "Integrating....."

This is not a prompt. It merely indicates that integration is currently under way.

G. "Touch space bar to continue, or mode select to stop"

If you have more samples to be analysed, do space bar.

H. "Same conditions as last run?" (yes or no) Type no if you want to change any options, such as peak number estimate.




EXAMPLE OF OUTPUT FROM ANALYSER

# INSTRUCTIONS ON OPERATION OF THE NUCLEUS/NORTHSTAR COMPUTER CONTROLLED SCANNING SCINTILLATION COUNTER

## I. INTRODUCTION

### A. Capabilities

This equipment will generate accurate, reproducable gamma scintillation spectra. The spectra may be saved on a mini-floppy diskette (one diskette will hold 65 spectra) for subsequent playback. The playback can be either to a strip chart recorder, graphics video terminal, or both.

After manual calibration of the Nuclear Analyser, the operator has control via video terminal of maximum and minimum scan energies, scan direction and chart recorder output width.

The software has been prepared in such a way as to be nearly self-teaching. A student can be taught to operate the equipment in just a few minutes.

Three switches located on the scintillation equipment can be set to give complete computer control or to give the "normal" original operation, completely independent of the computer. This is helpful in case of computer breakdown, which while rare, has been known to occur.

### B. Limitations

1. The "nuclear" equipment must still be calibrated manually.
2. Both ordinates (energy and amplitude) of chart recorder plotted spectra are limited to 256 points, due to the use of an 8 bit AD/DA converter to interface the computer with the "nuclear" equipment.
3. Amplitude and energy ordinates of video plots are limited to 24 and 80 points respectively.

### C. Hardware Description

This equipment can be visualized in three sections.

1. The scintillation equipment, consisting of: (Figure 1)
   a. detector
   b. pulse height analyser
   c. GM counter/scaler
   d. chart recorder
2. The computer equipment, consisting of: (Figure 2)
   a. Horizon II microcomputer
   b. Cromenco 8 bit AD/DA
   c. Lear Siegler video terminal
3. The interface hardware (Figure 3)

   The interface hardware consists of several operational amplifier circuits. The function of these circuits is to match the voltage levels of the scintillation equipment with the AD/DA converter in the computer.

## II. START-UP AND OPERATION OF SYSTEM

### A. Scintillation Equipment

1. Set the three extra toggle switches (SW 1-3) to their up positions. This gives total computer independence (Figure 4).
2. Tune up scintillation equipment in normal way.
3. Reset extra toggle switches as desired.

| SWITCH | SETTING | EFFECT |
|---|---|---|
| SW 1 | up | Internal chart adv |
| | down | Computer chart adv |
| SW 2 | up | Direct GM to recorder pen |
| | down | GM signal routed thru computer to recorder pen |
| SW 3 | up | Pulse height analyser scan ramp generated internally |
| | down | Pulse height analyser scan ramp generated by computer |

### B. Computer Equipment

1. Turn on computer and terminal.
2. Insert program (L.H. drive) and spectrum data (R.H. drive) disks.
3. Push reset switch on computer. You should see a message followed by a *.
4. Loading and execution of program
   a. Respond to * by typing: GO BASIC < cr >
   b. Respond to READY by typing: Memset 48000 < cr >
   c. Respond to READY by typing: load gamscn < cr >
   d. Respond to READY by typing: run < cr >
   e. If you have any trouble, remove disks, go to B1 and try again.

### C. Operation of Program

1. Study "help" file within program.
2. Attend instructors' lectures on operation.

FIGURE 1

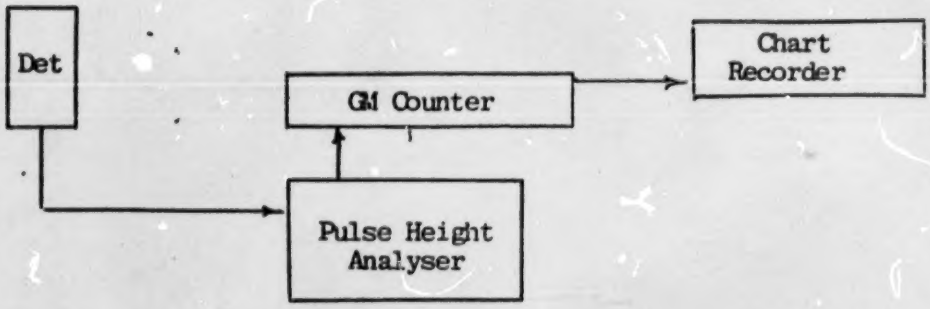



FIGURE 2

FIGURE 4

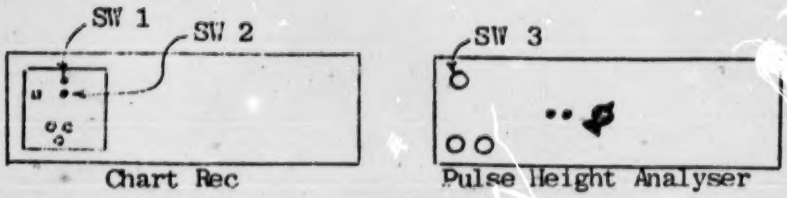
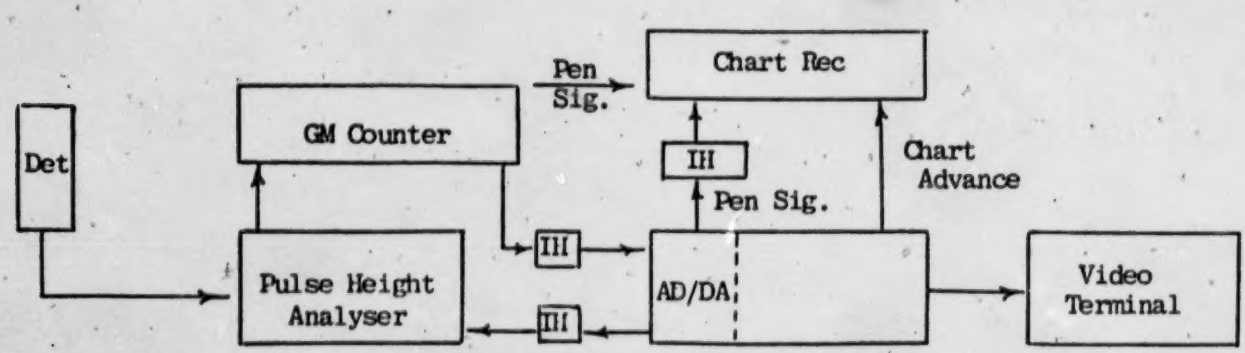
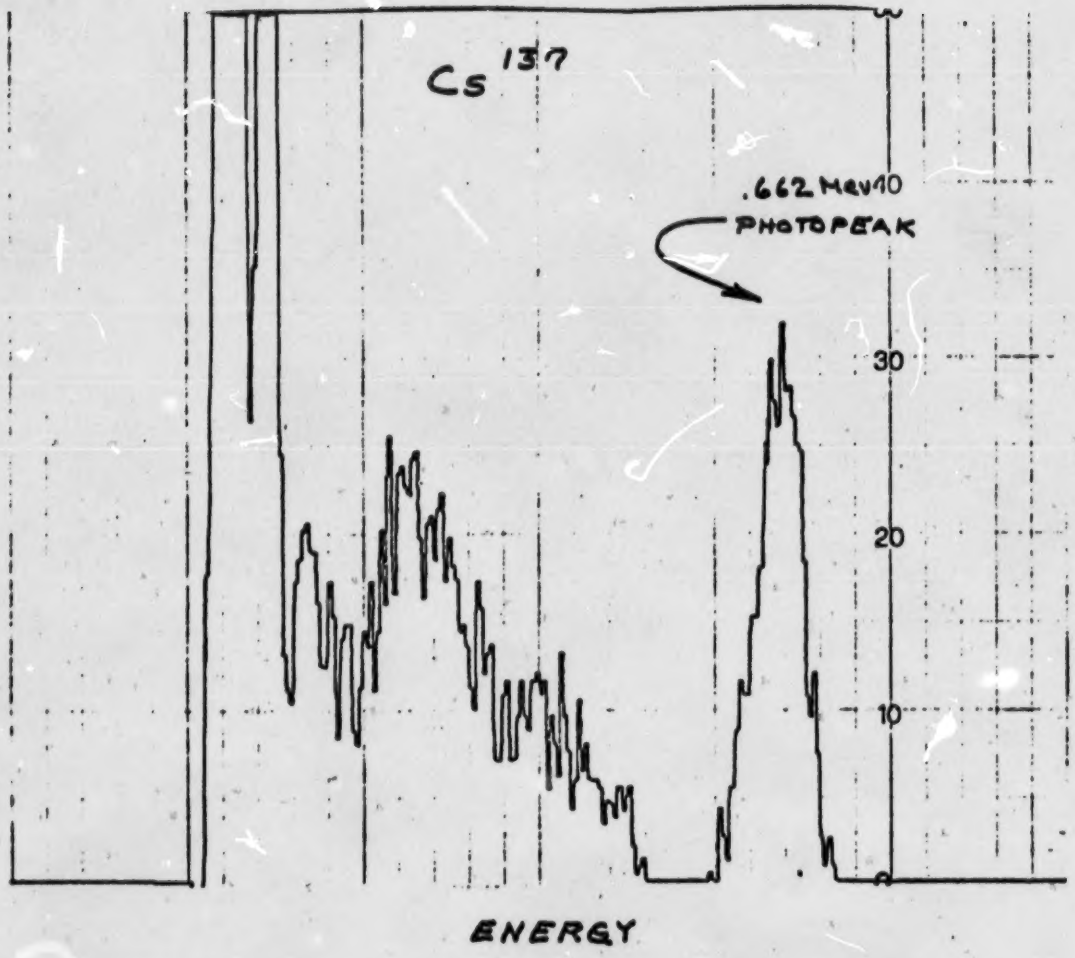


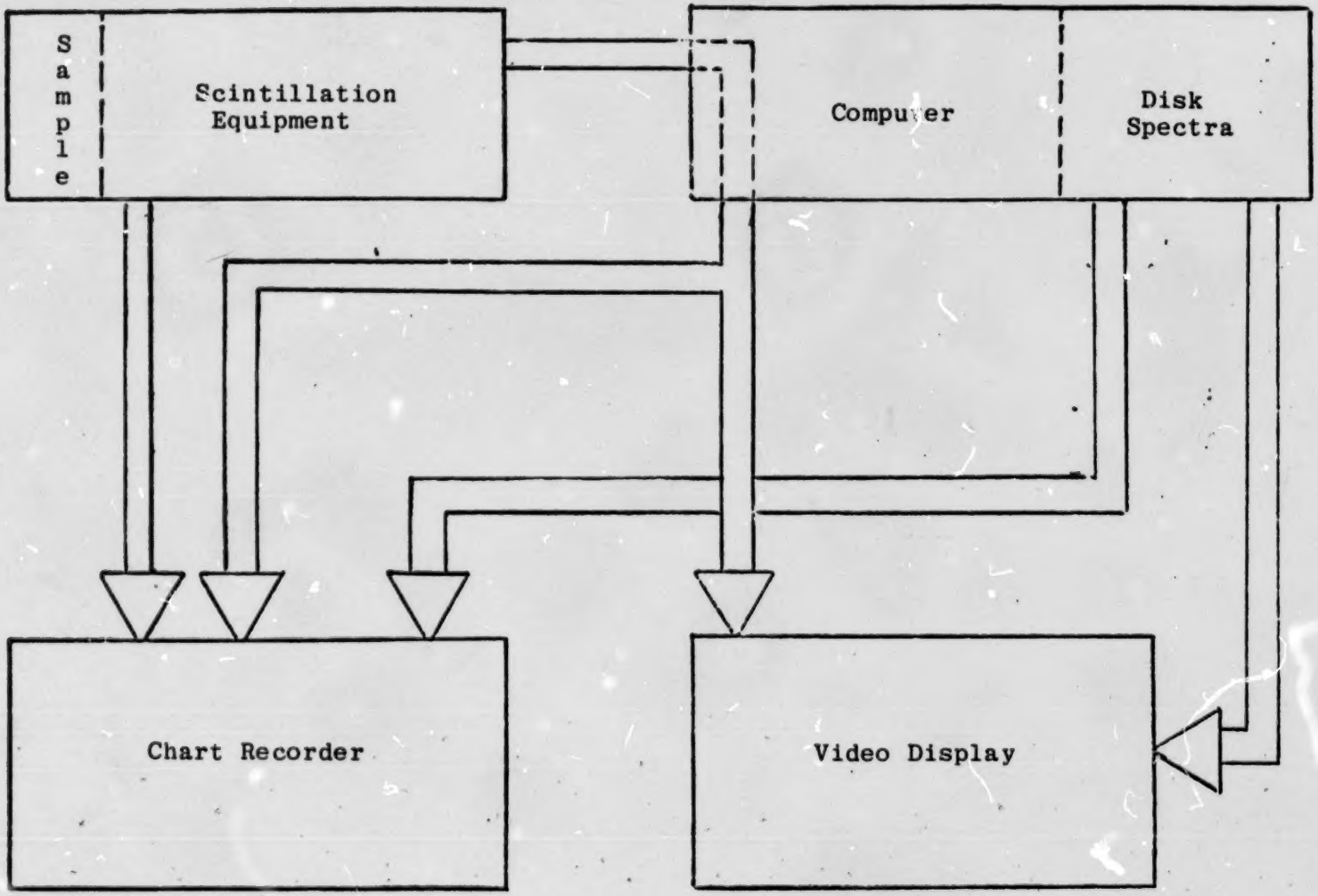

FIGURE 3

Boxes labeled IH are the interface hardware






EXAMPLE OF SCAN ON SCINTILLATION SPECTROMETER




INFORMATION PATHS AVAILABLE IN COMPUTER CONTROLLED SPECTROPHOTOMETER

INITIALIZATION

SELECTS SCAN CONDITIONS
SAMPLE VS DISK SCAN
PRINTER VS VIDEO PLOT
SCAN SPEED, DIRECTION,
ENERGY LIMITS

EXECUTIVE

DOES SCAN
(IF APPROPRIATE):
DRAWS AXES
PRINTS PROMPT LINE
READS RATEMETER
SAVES RATEMETER DATA
FOR POSSIBLE DISK SAVE

OUTPUTS RAMP TO ANALYZER
OUTPUTS TO CHART RECORDER:
PEN SIGNAL, PAPER ADVANCE SIGNAL

ABORTS, PAUSES, JUMPS TO END,
RESTARTS SCAN

END OF SCAN
SAVES SCAN, RESTARTS SCAN
NEW SCAN, QUIT

MAIN SUBROUTINES

HELP

NON-NORMAL SCAN PARAMETERS

LOW LEVEL GRAPHICS

READ DISK CONTENTS

DRAW AXES

SAVE SCAN IN DISK FILE

NORMAL SCAN PARAMETERS

LOAD SPECTRUM FROM DISK FILE